Phys 7440 Problem set 8
Due Wed. Oct. 29

1. The Wannier functions of a band are defined in terms of Bloch functions of the same band by:

\[ w(r - r_n) = N^{-1/2} \sum_k \exp(-ik \cdot r_n) \psi_k(r), \]

where \( r_n \) is a lattice point. \( \psi_k(r) \) states are the Bloch states |k>. 

(a) (15 points) Prove that Wannier functions about different lattice points \( m, n \) are orthogonal:

\[ \int dV w^*(r - r_n) w(r - r_m) = 0 \text{ if } n \neq m. \]

This orthogonality makes the functions often of greater use than atomic orbitals centered on different lattice sites, because the latter are not generally orthogonal.

(b) (15 points) The Wannier functions are peaked around the lattice sites. Show that for

\[ \psi_k(r) = N^{-1/2} e^{ikx} u_0(x) \]

the Wannier function is:

\[ w(x - x_n) = u_0(x) \frac{\sin[\pi(x - x_n)/a]}{\pi(x - x_n)/a} \]

for \( N \) atoms on a line of lattice constant \( a \).

2. Consider electrons on a two-dimensional square lattice in the tight-binding approximation with near-neighbor terms only.

a) (10 points) The band dispersion in the tight binding approximation with nearest-neighbor overlap only with the bottom of the band defined to be zero energy is:

\[ \varepsilon = \varepsilon_0 (2 - \cos(ak_x) - \cos(ak_y)). \]

What is \( \varepsilon_0 \) in terms of the wavefunctions \( \phi_s(r) \) of the s-orbitals and the potential \( \Delta U(r) \), which is the additional potential energy that comes from the interactions between an electron on a given site and neighboring sites.

b) (10 points) Show that one electron per site always implies that the area of the Fermi surface is \( \frac{1}{2} \) of the area of the Brillouin zone regardless of the precise band dispersion.

c) (5 points) With one electron per site in this crystal, draw the Fermi surface. (Hint: Use the result of (b) and the fact that the Fermi level must lie half way between the bottom and the top of the band.) Is this a metal or an insulator? In class we discussed that nesting of the Fermi surface occurs when the Fermi surface has parallel sheets (or lines in 2D) Is this Fermi surface nested or not?
d) (5 points) With one electron per site in this crystal draw a constant energy contour for an energy below the Fermi energy.

e) (5 points) With one electron per site in this crystal draw a constant energy contour for an energy above the Fermi energy.

3. (25 points) Compare the result of prob. 1b in problem set 6 for the lowest NFE energy band to the result found in class for tight binding $S$-band on a cubic lattice:

$$\epsilon_k^{T,B} = \epsilon^0 - \beta - 2\gamma(\cos(k_xa) + \cos(k_ya) + \cos(k_za))$$

Assume the energy zero at the $\Gamma$-point is the same for both the NFE and the tight binding models and that the tight binding effective mass, $\frac{\hbar^2}{2t_1a^2}$ is equal to the free electron mass. What values of $U_k$ must be used at the X and W points to bring the NFE and tight binding bands into agreement at X and W. Are these values consistent with a 'weak periodic potential'? Discuss the following question: For a material of typical lattice spacing, $a=2\text{Å}$ is it ever likely that a tight binding calculation could yield $m^*=m$ and remain valid?

(Hint: You will need to adjust the values of $U_1$, $U_2$ and $U_3$ to make the dispersion of the lowest band in prob. 2b as close to the tight binding result as possible by expressing them in terms of $t_1$ and $\epsilon^0$.

1. Match the zeros of energy, 2. Match the curvature at $\Gamma$, 3. Match the energies at X, 4. Match the energies at W.)